Confinement-deconfinement transition in a generalized Kitaev model.

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We present a spin model, namely, the Kitaev model augmented by a loop term and perturbed by an Ising Hamiltonian and show that it exhibits both confinement-deconfinement transitions from spin liquid to antiferromagnetic/spin-chain/ferromagnetic phases and topological quantum phase transitions between gapped and gapless spin liquid phases. We develop a Fermionic mean-field theory to chart out the phase diagram of the model and estimate the stability of its spin liquid phases which might be relevant for attempts to realize the model in optical lattices. We also conjecture that some of the confinement-deconfinement transitions in the model, predicted to be first order within the mean-field theory, may become second order via a defect condensation mechanism.

Quantum phase transition from ordered to paramagnetic phases in two-dimensional (2D) spin models has been a subject of recent interest[1]. Such paramagnetic phases and associated quantum phase transitions have been conjectured to be of relevance to the properties of several strongly correlated systems including cuprates and quasi-2D organic materials [2, 3, 4]. A class of these paramagnetic phases which do not break any constituent symmetries of their underlying lattice are called spin-liquids and are generally believed to be natural candidates for paramagnetic phases obtained by disordering non-collinear spin-ordered magnets [5]. However, the precise criteria for realization of spin liquids and the nature of quantum phase transitions to them from spin-ordered phases are far from being settled issues [6]. The physics of these spin-liquid phases can be described by representing the spins in terms of spinons, which are Fermionic $CP(N)$ fields, coupled to bosonic gauge fields [2, 5]. In most commonly studied examples, the symmetry group associated with these gauge fields are either $U(1)$ or Z_2; the corresponding spin-liquids being dubbed as $U(1)$ or Z_2 spin liquids. In the ordered phase of spins, the spinons are confined while the spin-liquid paramagnets constitute phases with gapped or gapless deconfined spinon excitations. Thus the transition between these phases serve as examples of confinement-deconfinement transitions for spinons. Examples of such transitions has been studied in several high energy and condensed matter models [7, 8, 9].

In this letter, we present a spin model, namely the Kitaev model augmented by a loop term and perturbed by an Ising model, on a 2D hexagonal lattice with the Hamiltonian

$$H = H_K + H_L + H_I, \quad H_K = -\sum_{j \in A} \sum_{\alpha\,link} J_\alpha \sigma_j^\alpha \sigma_{j'_\alpha}^\alpha$$

$$H_I = \lambda J \sum_j \sum_{all\,links} \sigma_j^z \sigma_{j'}^z, \quad H_L = -\kappa J \sum_p W_p \quad (1)$$

where j'_α is the nearest neighbor of j connected by the $\alpha = x, y, z$ link of the hexagonal lattice as shown in Fig. 1, σ^α are the usual Pauli matrices, $W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$ is the loop operator, where, as shown in Fig. 1, 1..6 denotes sites of a hexagonal plaquette, A and B denotes two sublattices of the honeycomb lattice, and j' denotes all nearest neighbors of j. We demonstrate that this model exhibits confinement-deconfinement transitions from deconfined spin liquid to confined Ising ordered antiferromagnetic (AFM), ferromagnetic (FM) or spin-chain (SC) phases and can therefore serve as a test bed to study such transitions. In addition, we show that the model also supports two distinct spin liquid phases with gapped and gapless deconfined spinon excitations and exhibits a topological quantum phase transition between them. To the best of our knowledge, the model presented here is the only spin model which supports spin liquid phases with both gapped and gapless deconfined spinon excitations and displays both confinement-deconfinement and topological quantum phase transitions. We chart out the phase diagram of this model using a Fermionic mean-field theory and estimate the stability of the deconfined phases as a function of the strengths of the loop and Ising terms. There have been proposals for experimentally realizing the Kitaev model in systems of ultracold atoms and molecules trapped in optical lattices [15]. Any such physical realization of this model will always have contaminating interactions; our work thus provides an estimate of the stability of its gapless spin liquid phase against such interactions. Finally, we conjecture that the confinement-deconfinement transition between the gapped deconfined Kitaev phase and the confined Ising AFM or FM phases, predicted to be first order within the mean-field theory, may turn out to be second order via a defect condensation mechanism at large κ.

The Kitaev model with Hamiltonian H_K is a rare example of a 2D spin model which can be exactly solved [10, 11, 12, 13, 14]. The ground state of the model, for
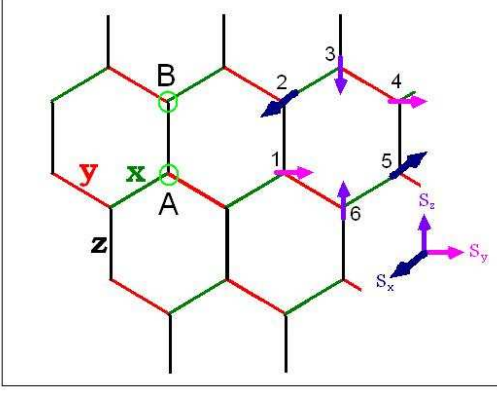
FIG. 1: (Color online) Schematic representation of the Kitaev model on a honeycomb lattice showings the different links x, y and z and the two sublattices A and B. The sites labeled 1..6 and their spin configuration is a schematic representation for a classical configuration with $\langle W_p \rangle = 1$

the parameter regime $|J_1 - J_2| \leq J_3 \leq J_1 + J_2$, supports a gapless phase [10] which can be described as a Z_2 spin liquid constituting a Fermi sea of deconfined gapless spinons and static Z_2 gauge fields. These spinons become gapped beyond this regime. Both the gapped and the gapless spinon phases have unit expectation value for a non-local loop operator W_p: $\langle W_p \rangle = 1$. They are distinguished by the value of the Chern number which is ± 1 for the gapless phase and 0 for the gapped phases.

In the present work, we study the effect of augmenting the Kitaev model with a loop term and perturbing it with an Ising Hamiltonian. In what follows, we shall study the Kitaev model in the isotropic limit and scale all energies by J: $J_\alpha = J = 1$ and obtain the phase diagram of H as functions of dimensionless couplings κ and λ. We note at the outset, that the ground state of the system at $\lambda = 0$ is the Kitaev ground state with gapless deconfined Fermionic spinons coupled to a frozen gauge field configuration. This ground state is exactly captured by the Fermionic theory which makes it an ideal starting point for our analysis. The ground state of the system at $\lambda \rightarrow \pm\infty$ is the Ising AFM/FM which are magnetically ordered phases with confined spinons. Thus the model, by construction, clearly supports confinement-deconfinement transitions.

We begin by mapping the spin model H to a Fermionic model H_F, by using the Jordan-Wigner transformations [12]. We choose a path $\{i(n)\}$ which runs along the x and y bonds and define $\sigma^z_{j(n)} \equiv ic_{j(n)}b^z_{j(n)}$, $\sigma^x_{j(2n)} \equiv c_{j(2n)} \prod_{m<2n} \sigma^z_{k(m)}$, $\sigma^x_{j(2n+1)} \equiv b^z_{j(2n+1)} \prod_{m<2n+1} \sigma^z_{k(m)}$, and $\sigma^y_j = i\sigma^x_j \sigma^z_j$, where c_j, b^z_j are Majorana fermions operators at site j [$(j(2n), j(2n-1))$ are the x bonds and $(j(2n+1), j(2n))$ are the y bonds]. The resultant

Hamiltonian becomes

$$
\begin{aligned}
H_F &= -\sum_{j \in A} \Big[\sum_{\alpha=x,y\,links} ic_j c_{j'_\alpha} + \sum_{z\,link} ib^z_j c_j ib^z_{j_z} c_{j'_z} \Big] \\
&\quad -\kappa \sum_{j,k \in plaquette} \sum_{z link} ib^z_j b^z_{j_z} ib^z_k b^z_{k'} \\
&\quad +\lambda \sum_j \sum_{\alpha=all\,links} ib^z_j c_j ib^z_{j_\alpha} c_{j'}
\end{aligned}
\tag{2}
$$

where the subscript $j, k \in plaquette$ indicates that the sum is over sites which belong to the A sublattice of a given plaquette as schematically shown in Fig. 1. Note that for $\lambda = 0$, the operators $ib^z_j b^z_{j_z}$, commute with the Hamiltonian and are therefore a constants of motion. In this limit, H is exactly solvable. When λ is turned on, these operators acquire dynamics and their fluctuations are ultimately expected to confine the spinons through a confinement-deconfinement transition.

To make further progress, we treat H_F within an RVB type mean-field theory [2] and introduce the mean-fields on the sites (corresponding to spin ordering) and on links (corresponding to the emergent gauge fields) of the hexagonal lattice: $\langle ib^z_j c_j \rangle = \langle \sigma^z_j \rangle = \Delta_{1(2)}$, $\langle ib^z_j c_{j'} \rangle = \beta_\alpha$, $\langle ib^z_j b^z_{j_\alpha} \rangle = \gamma_\alpha$, and $\langle ic_j c_{j'_\alpha} \rangle = \gamma_{0\alpha}$. Note that keeping in mind the bipartite nature of the hexagonal lattice and to allow for possible AFM phases, we have introduced two mean-fields Δ_1 and Δ_2 corresponding to the two sublattices shown in Fig. 1. In terms of these mean-fields, one can decompose the quartic terms in H_F as

$$
\begin{aligned}
ib^z_j b^z_{j_z} ib^z_k b^z_{k'_z} &= i\gamma_z(b^z_j b^z_{j_z} + b^z_k b^z_{k'_z}) - \gamma^2_z \\
ib^z_j c_j ib^z_{j_\alpha} c_{j'} &= \gamma_\alpha ic_j c_{j'_\alpha} + \gamma_{0\alpha} ib^z_j b^z_{j_\alpha} - \gamma_\alpha \gamma_{0\alpha} \\
&\quad -\Delta_1 ib^z_{j_\alpha} c_{j'_\alpha} - \Delta_2 ib^z_j c_j + \Delta_1 \Delta_2 \\
&\quad -i\beta_\alpha(b^z_j c_{j'} + b^z_{j_\alpha} c_j) - \beta^2_\alpha,
\end{aligned}
\tag{3}
$$

where we have only considered mean-fields which are either on-site or reside on links between two neighboring sites. The resultant quadratic mean-field Hamiltonian, in momentum space, can be written as

$$
\begin{aligned}
H_{\mathrm{mf}} &= \frac{1}{N} \sum_{\vec{k}} \Big[J_0 \Big(\alpha + e^{ik_1} + e^{i(k_1+k_2)} \Big) c^{A\dagger}_{\vec{k}} c^B_{\vec{k}} \\
&\quad + J'_0 \Big(\beta - 2\kappa\gamma_z/J'_0 + e^{ik_1} + e^{i(k_1+k_2)} \Big) b^{A\dagger}_{\vec{k}} b^B_{\vec{k}} \\
&\quad + (ic^{A\dagger}_{\vec{k}} b^B_{\vec{k}} - ib^{A\dagger}_{\vec{k}} c^B_{\vec{k}})(\beta_z(1+\lambda) + \beta_x e^{ik_1} \\
&\quad + \beta_y e^{ik_2}) - c_1 b^{A\dagger}_{\vec{k}} c^A_{\vec{k}} - c_2 b^{B\dagger}_{\vec{k}} c^B_{\vec{k}} + \mathrm{h.c} \Big] \\
&\quad + \kappa\gamma^2_z - (1+\lambda)\gamma_z\gamma_{0z} + (1+3\lambda)\Delta_1\Delta_2
\end{aligned}
\tag{4}
$$

where $J_0 = (1 + \lambda\gamma_x)$, $\alpha J_0 = (1+\lambda)\gamma_z$, $J'_0 = \lambda\gamma_{0x})$, $\beta J'_0 = (1+\lambda)\gamma_{0z}$, $c_{1(2)} = (1+3\lambda)\Delta_{1(2)}$, and the momentum $\vec{k} = k_1 \hat{e}_1 + k_2 \hat{e}_2$ with the unit vectors $\hat{e}_1 = \hat{x} + \hat{y}/\sqrt{3}$ and $\hat{e}_2 = 2\hat{y}/\sqrt{3}$.

We now minimize H_{mf} numerically and obtain the mean-field phase diagram of the model as a function of
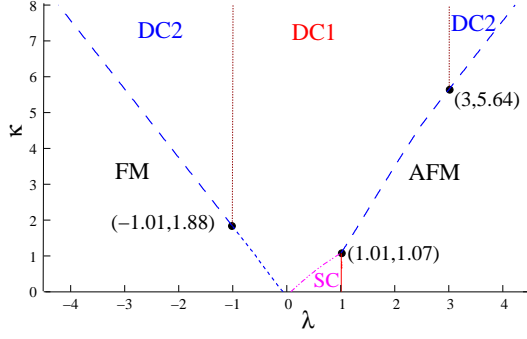
FIG. 2: (Color online) The mean-field phase diagram for the model. The blue dashed lines represent confinement-deconfinement transitions which may become second order via defect condensation mechanism. The triple points occur at $(\lambda_1^*, \kappa_1^*) = (1.01, 1.07)$ and $(\lambda_2^*, \kappa_2^*) = (3, 5.64)$ for $\lambda > 0$ and $(\lambda_3^*, \kappa_3^*) = (-1.01, 1.88)$ for $\lambda < 0$.
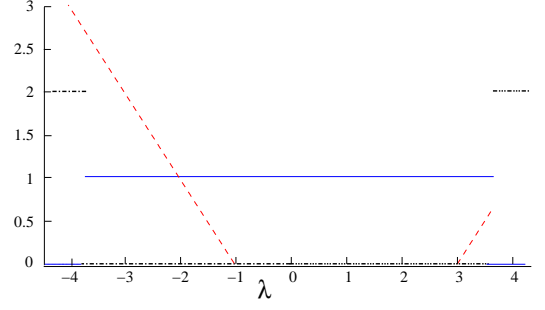

FIG. 3: (Color online) Plot of the loop order parameter (solid blue line), the spinon gap (red dashed line) and the FM and the AFM order parameters (black dash-dotted lines) as a function of λ for $\kappa = 7$.

λ and κ. Note that the mean field solution is exact at $\lambda = 0$. This phase diagram is shown in Fig. 2. In accordance with our earlier expectation, we find that at large positive (negative) λ, the ground state of the model is an Ising AFM (FM) which corresponds to confined phase of spinons while at small λ, the model exhibits a deconfined gapless phase DC1. The transition between these two phases at low κ and for positive λ occurs via a SC phase, which corresponds to AFM alignment of spins along chains in x direction of the hexagonal lattice with ferromagnetic arrangement of such chains in the y direction. For negative λ, there is a direct transition to the FM phase. At high enough values of κ, we find another gapped deconfined phase DC2 and second order topological quantum phase transitions between DC1 and DC2 phases. The confinement-deconfinement transitions at high κ always occur from DC2 to AFM/FM phases. These transitions are predicted to be first order within mean-field theory. The phase diagram exhibits two triple points at $(\lambda_1^*, \kappa_1^*) = (1.01, 1.07)$ and $(\lambda_2^*, \kappa_2^*) = (3, 5.64)$ for $\lambda > 0$. These represent meeting points of AFM, SC and DC1 and AFM, DC2 and DC1 phases respectively. For $\lambda < 0$, there is one triple point $(\lambda_3^*, \kappa_3^*) = (-1.01, 1.88)$ where the FM, DC1, and DC2 phases meet. We also note that our mean-field analysis also gives an estimate for the stability of the deconfined phase of the Kitaev model ($-0.07 \leq \lambda_c \leq 0.08$ for $\kappa = 0$) under external perturbing Ising term which may be important for physical realization of the Kitaev model and for quantum computing proposals based on it [15, 17].

The plot of the loop order parameter $\langle W_p \rangle$, the spinon gap, and the AFM and the FM order parameters as obtained from the mean-field theory, is shown, for $\kappa = 7$, as a function of λ in Fig. 3. We note that all the order parameters show discontinuous changes at the transition points indicating first order transitions. The spinon gap, in contrast, increases linearly and continually with λ in-

dicating a second order quantum phase transition between DC1 and DC2 phases. The presence of this topological quantum phase transition and the linear variation of the spinon gap with λ can be understood qualitatively from H_{mf}. For large κ, it requires a large λ to destabilize the Kitaev ground state in favor of Ising AFM/FM. In addition, numerically we find that in the Kitaev phase $\gamma_z(\gamma_x) \sim 1(0)$. As a result, beyond a critical value of $\lambda = \lambda_c$, the effective couplings along the links, $J_{1,2} \sim (1 + \lambda\gamma_x)$, $J_3 \sim \gamma_z(1 + \lambda)$, fail to satisfy $|J_1 - J_2| \leq J_3 \leq J_1 + J_2$ thus leading to a gapped phase via a topological quantum phase transition [10, 11]. The spinon gap in this gapped phase varies linearly with J_3 [11, 14] and hence shows a linear variation on λ. At small κ, the confinement-deconfinement transitions to the SC/FM phases occur before λ_c is reached and hence the topological phase transitions do not occur.

Next, we argue that it is possible that some of the confinement-deconfinement transitions, predicted to be first order by mean-field theory, can become second order in the large κ limit via a defect condensation mechanism [18]. We note that similar second-order transitions have been seen in numerical studies of related models [16, 19]. We begin with the case $\lambda > 0$ and start from the Ising AFM ground state. The possible classical defect spin configurations over this ground states whose condensation can lead to either the Kitaev or the SC phases are shown in Fig. 4. The energy of these defects are given by $E_{sc} = 8(\lambda - 1)$, $E_{DC1} = 14\lambda - 6 - \kappa$, and $E_{DC2} = 10\lambda - 2 - \kappa$. Note that $E_{AFM} = E_{DC1} = E_{sc} = E_{DC2} = 0$ at $\lambda = \lambda^* = 1$ and $\kappa = \kappa^* = 8$ which represents a triple point in the $\kappa - \lambda$ plane. For the SC phase to occur, we need $E_{sc} = 0$ and $E_{sc} \leq E_{DC1}, E_{DC2}$ which yields the conditions

$$\lambda_c^{sc} = 1 \quad \kappa_c^{sc} \leq 6\lambda + 2, \quad \kappa_c^{sc} \leq 2\lambda + 6 \qquad (5)$$

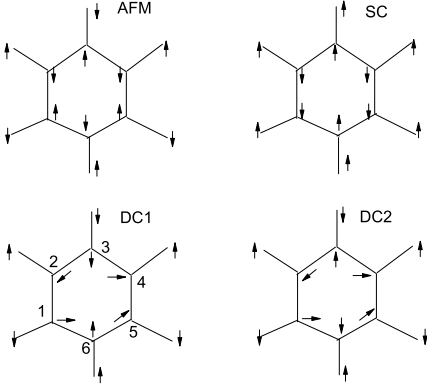Similar analysis lead to conditions for instability due to

FIG. 4: Schematic representation of classical spin configuration of the AFM phase and possible defects that can destabilize this phase. See text for details.

condensation of the defects DC1 and DC2:

$$\lambda_c^{DC1} = \frac{\kappa_c^{DC1}}{14} + \frac{3}{7} \quad \lambda_c^{DC1} \leq 1, \quad \kappa^{DC1} \geq 6\lambda + 2, \quad (6)$$

$$\lambda_c^{DC2} = \frac{\kappa_c^{DC2}}{10} + \frac{1}{5} \quad \lambda_c^{DC2} \geq 1, \quad \kappa^{DC2} \geq 2\lambda + 6. \quad (7)$$

From Eqs. 5, 6, and 7, we find that the SC phase destabilize the AFM phase at $\lambda = 1$ for all $\kappa \leq \kappa^*$. This represents an order-order transition which is expected to be first order. As we decrease λ further below 1, the deconfined gapless Kitaev phase takes over at some point. The nature of this transition is not predictable from this condensation mechanism, since the transition do not take place from the AFM phase. For $\kappa \geq \kappa^*$, the AFM phase is destabilized in favor of the deconfined phase DC2 when $\lambda^c = \kappa^c/10 + 1/5$. The DC2 phase represents a disordered phase in terms of the spin variables and thus this transition can be second order. For $\kappa > \kappa^*$, the energy of DC1 becomes lower than that of DC2 for $\lambda \leq 1$. This indicates a second order transition between the two deconfined phases with no broken symmetries and is therefore a the topological quantum phase transition. Note that this transition line is independent of κ and therefore is expected to appear as a vertical line in the $\kappa - \lambda$ plane. A similar discussion for $\lambda < 0$ shows that the defect condensation energies of the phases DC1 and DC2 (the SC phase is not energetically favorable for $\lambda < 0$) over the FM state are $E'_{DC1} = 14|\lambda| + 6 - \kappa$ and $E'_{DC2} = 10|\lambda| + 2 - \kappa$. We find that such a mechanism works only for large κ where E'_{DC1} and E'_{Dc2} can be negative and in this regime the FM phase is always destabilized by the DC2 phase leading to a confinement-deconfinement at $|\lambda| = \kappa/10 - 1/5$. For lower κ, we expect to find a transition between the DC1 and the FM phase which is not mediated by such defect condensation. The phase diagram obtained by this simple qualitative discussion of the defect condensation mechanism described above has most of the major features shown in Fig. 2 and a direct AFM to DC1 transition line at intermediate κ for $\lambda > 0$) and this gives us

some confidence about it's qualitative correctness [20]. A quantitatively accurate study of the obtained phase diagram requires a more sophisticated treatment of quantum fluctuations and is left for future study.

To conclude, we have presented a spin model, namely the Kitaev model, augmented by a loop term and perturbed by an Ising Hamiltonian, and have shown that the model exhibits a rich phase diagram with both confinement-deconfinement and topological quantum phase transitions. We have estimated that the topological phase of the Kitaev model is unstable to about 10% contamination by Ising interactions.

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